"Structural and Dynamics Behavior of Nitriles through Dielectric Properties using a Time Domain Reflectrometry (TDR)"

Synopsis

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By

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Abstract of proposed work plan/problem

"Structural and Dynamics Behavior of Nitriles through Dielectric Properties using a Time Domain Reflectrometry (TDR)"

1. Introduction

The force that holds atoms together within the molecules is called intermolecular force. These intermolecular forces play a vital role in the formation of mixture. A solution is formed when one substance dissolves in to another substance. A solution is a homogeneous mixture of two entities namely called as solute and solvent. The solute is the substance that is being dissolved, while the solvent is the dissolving medium. Solutions can be formed with many different types and forms of solute and solvents. The simplicity with which solute molecules take the position of solvent molecules depends on the relative potential of three types of interactions; Solvent - solvent, Solute – solute and Solvent– solute. The solution contains molecules with electropositive hydrogen with electronegative atom (like nitrogen, oxygen, sulfur, or fluorine), the properties of the solution changes extremely due to hydrogen bonding [1-5]. Hydrogen bonds may form between similar molecules or in between different molecules.

For present study the nitriles are chosen as a solute. Nitriles are a class or category of chemical compounds that include a nitrogen atom connected to a carbon atom by a triple covalent bond. Nitrile molecules can vary in size up to very long molecules most of which consist of carbon atoms attached to each other and also to hydrogen atoms. Nitriles are polar organic liquids with a large dipole moment the intermolecular interactions are strong and can cause association of the molecules. The main interest of study to understand non-hydrogen

bonded aprotic solvent in non-polar solute (like dioxane) which provides information about breaking of molecular multimer structures in the system.

Time Domain Dielectric relaxation spectroscopy is one of the most popular spectroscopy having frequency range from 10^{-4} Hz to 10^{12}Hz. So this spectroscopy is known as broadband dielectric spectroscopy. The Time domain dielectric relaxation spectroscopy has very sensitive relaxation process for an extremely wide range of time i.e. $10^{5} – 10^{-12}$ sec. Dielectric spectroscopy is used to understand the various terms like interaction between solute –solvent, charge distribution, orientation of molecules [6-9].

Purpose of present work is to study dielectric relaxation and structural and dynamic behavior of nitriles in aprotic solvent like 1,4-Dioxane using TDR technique. Time Domain Reflectometry' (TDR) measurement technique will be used to study the various properties of Nitriles also used to determine the dielectric properties of the material such as Static dielectric constant (ε0) , dielectric constant (ε,), dielectric loss (ε") and dielectric Relaxation time(τ).

2. Literature Review and Development in the Subject(previous work done in the relevant area):

In recent years, dielectric measurements have become an effective tool for extracting significant information related to the structure and to the quality-status of various materials: The following scientists are actively doing research in this field at international/National level:

International/National status:

Kadaba et al studied some nitriles at microwave frequency near room temperature and also studied dielectric relaxation of nitriles with some substituted benzenes [10]. Flueckinger et al have been measured dielectric constant of some liquid nitriles. The dielectric data were analyzed

on the basis of an equilibrium between monomer and an antiparallel dipole pair dimer, and the nature of the association is discussed [11]. Dielectric constants and losses have been measured at 30^{o}C by Prasad et. al.[12] . The complex dielectric function, ionic conductivity and impedance behavior of acetonitrile have been investigated over the frequency range 20 Hz-1 MHz and at the different temperatures by Sengwa et. al.[13]. In this field, many scientific efforts have been done to the dielectric spectroscopy of liquids. There is great interest to study the dielectric relaxation behavior in polar system to understand the molecular structure and dynamics of polar liquid with modification of molecular structure due to the presence of polar or non-polar molecules. Some considerable experimental studies about the dielectric relaxation behavior of liquids solutions of n-nitriles have been reported.[14-16].Mehrotra *et.al*. [17] also developed the TDR measurement in India for the measurement of polar and non-polar solutions. The earlier experimental analysis on nitriles gives information regarding relaxation time and solute solvent interactions [18-23].

3. Objective of research/Proposed Hypothesis:

- To determine complex permittivity of Nitriles using Time Domain Reflectometry Technique.
- To determine static dielectric constant, dielectric loss and relaxation time at high frequency.
- To determine the Excess dielectric Permittivity.
- To study molecular interaction and hydrogen bonding of solvents through various parameters like Krikwood correlation factor, Bruggman factor, Thermodynamic Prametrs, Excess parameters etc. using picoseconds dielectric relaxation spectroscopy

4. Methodology to be adopted:

Time Domain Reflectometry (TDR) technique is very much useful for measurement of complex permittivity spectra in broad range of frequencies in single measurement.. The Tektronix model no. DSA8300 Digital Serial Analyzer sampling mainframe along with the sampling module will be used for the time domain reflectometery (TDR). Figure 1 shows experimental setup for TDR. A repetitive fast rising 250mV voltage pulse of 200 KHz with 12ps incident and 15ps reflected rise time was fed through coaxial line system of impedance 50 ohm. Sampling oscilloscope monitors changes in step pulse after reflection from the end of line. Reflected pulse without sample $R_1(t)$ and with sample $R_x(t)$ will be recorded in time window of 5ns and digitized in 2000 points.

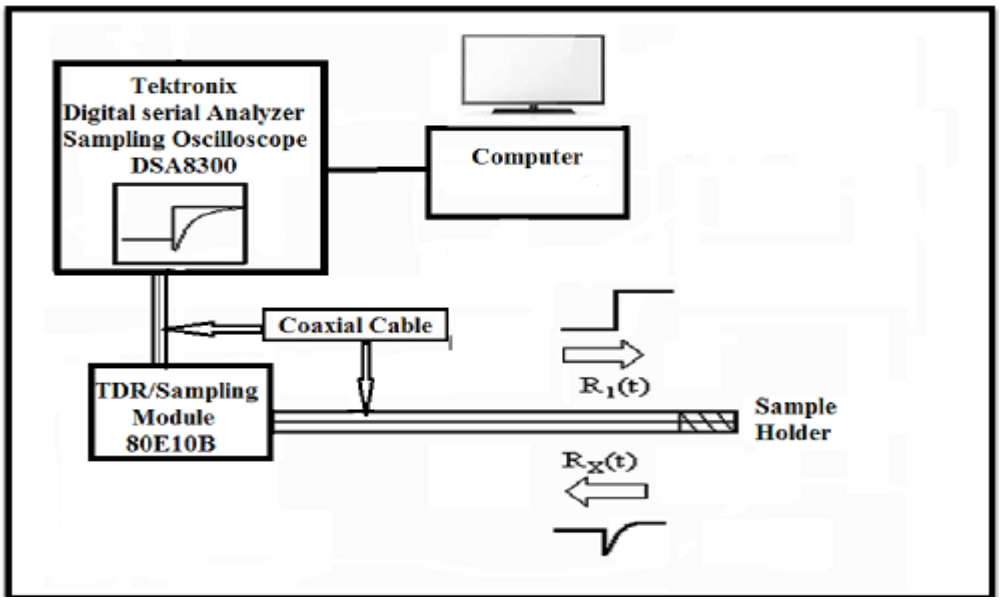

Fig1. Block diagram of Time Domain Reflectometry..

5. Importance of study/society application

There is great interest to study the dielectric relaxation behavior in polar system to understand the molecular structure and dynamics of polar liquid with modification of molecular structure due to the presence of polar or non-polar molecules. Nitriles are polar organic liquids with a large dipole moment. Due to large dipole moment the intermolecular interactions are strong and can cause association of the molecules. Dielectric studies of nitriles were studied because (i)nitriles exist in the liquid state at room temperature (ii) they are non-hydrogen bonded and (iii) they have large dipole moment. Nitriles are found in many useful compounds, including methyl cyanoacrylate, used in super glue, and nitrile rubber, a nitrile-containing polymer used in latex-free laboratory and medical gloves. Nitrile rubber is also widely used as automotive and other seals since it is resistant to fuels and oils. Nitriles are highly polar aprotic liquids which are widely used as industrial solvents; some of the nitriles are also pharmaceutically important. These systems are non-hydrogen bonded systems with large values of dipole moments.1,4-Dioxane having dipole moment 0.45D.1,4-Dioxane is used as a versatile aprotic solvent for ink adhesives and cellulose esters.

- **Significance of the study:**

  The present study is devoted to dielectric relaxation of nitriles in non-hydrogen bonded solvent like 1,4 Dioxane using TDR technique from 10MHz to 30GHz. from dielectric relaxation parameters; and understand orientation through solute-solvent interactions. There will be great interest to study the dielectric relaxation behavior in polar system to understand the molecular structure and dynamics of polar liquid with modification of molecular structure due to the presence of polar or non-polar molecules. Nitriles are

polar organic liquids with a large dipole moment. Due to large dipole moment the intermolecular interactions are strong and can cause association of the molecules. Dielectric studies of nitriles were studied because (i)nitriles exist in the liquid state at room temperature (ii) they are non-hydrogen bonded and (iii) they have large dipole moment.

6. Proposed work plan/Formulation and structure of study:

First Year: Literature survey, understanding of experimental setup , Chemicals collection & solvents selection for experimental work.

Second Year: Study of Dielectric measurement of following nitriles and also determine the dielectric parameters such as static dielectric constant, relaxation time, dielectric constant at high frequency and Kirkwood correlation factor.

Acetonitrile, Propionitrile ,Butyronitrile ,Pentanenitrile ,Hexaanenitrile,

Heptanitrile, Octanenitrile, Nanonitrile, Decanenitrile

Third year: (I) Paper presentation in the International/National Conference.

(ii) Writing research Paper and publish paper in the International Journals.

(iii) Thesis Writing and submission.

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Research Student	Research Guide
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